Revisiting numerical real-space renormalization group for quantum lattice systems

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Although substantial progress has been achieved in solving quantum impurity problems, the numerical renormalization group (NRG) method generally performs poorly when applied to quantum lattice systems in a real-space blocking form. The approach was thought to be unpromising for most lattice systems owing to its flaw in dealing with the boundaries of the block. Here the discovery of intrinsic prescriptions to cure interblock interactions is reported which clears up the boundary obstacle and is expected to reopen the application of NRG to quantum lattice systems. While the resulting RG transformation turns out to be strict in the thermodynamic limit, benchmark tests of the algorithm on a one-dimensional Heisenberg antiferromagnet and a two-dimensional tight-binding model demonstrate its numerical efficiency in resolving low-energy spectra for the lattice systems.

Since the success in solving the Kondo problem by Wilson [1], there had been lots of attempts in applying the numerical renormalization group (NRG) method to treat other quantum many-body problems in a similar way. However, the numerical RG algorithm based on real-space schemes met its Waterloo as it performed very poorly in subsequent several applications. In particular, the approach was shown to give inaccurate results for most interacting lattice systems [2–4] and for the Anderson localization problem [5, 6]. The difficulty, identified by White and Noack [7] via a simple one-dimensional tight-binding model, lies in that the approach is flawed in its treatment of boundaries of a block.

The inability to apply the NRG method to quantum lattice systems is a heavy loss to the research of condensed matter physics. Although a closely related method, the density matrix RG algorithm [8–10], was proposed later and has been shown very effective in achieving the ground-state energy for interacting lattice systems, there exist strong restrictions of this method in its application to excitation spectra or to systems with high spatial dimensions. The aim of this letter is to show that the flaw of the NRG method exposed previously can be eliminated via intrinsic prescriptions to cure interblock interactions and the derived "regularized" real-space blocking version of the NRG scheme is able to yield reliable results for quantum lattice systems.

In the standard real-space version of the NRG approach, one starts from a block Hamiltonian H_L of L sites and diagonalizes it exactly. By keeping a certain amount of the lowest-energy states $\{|\psi_j\rangle, j = 1, \cdots, m\}$, one then uses them to construct a Hamiltonian for a larger system composed of two such blocks: $H_{2L} = H_L^{[1]} + v_{12} + H_L^{[2]}$, where v_{12} denotes the interblock coupling. The primitive algorithm through projecting H_{2L} simply onto m^2 tensor product states $|\psi_j\rangle \otimes |\psi_{j'}\rangle$ fails to achieve reliable results. The new version of the NRG scheme here adopts a slightly different route: one should start by diagonalizing a pair of block Hamiltonians, e.g., the one H_L with an open boundary condition and the one with

a periodic form, H_L^p. Let us denote correspondingly the low-lying eigenstates of H_L^p by $\{|\psi_j^p\rangle\}$. The effective performance of the NRG algorithm resides in that, instead of using the set of tensor product states, the new pair of compound Hamiltonians, the open H_{2L} and the periodic $H_{2L}^p = H_{2L} + v_{21}$, are constructed and diagonalized in virtue of the following two sets of m^2 states

$$|\Psi_{jj'}\rangle = U_{adj} : |\psi_j\rangle \otimes |\psi_{j'}\rangle, \tag{1}$$

and

$$|\Psi_{jj'}^p\rangle = U_{adj}^{\otimes 2} : |\psi_j\rangle \otimes |\psi_{j'}\rangle, \tag{2}$$

respectively. The transformation U_{adj} here is the key prescription introduced to cure the interblock coupling. It is formally a range-L operator acting on adjacent segments of the compound block, namely, on the sites from $\frac{1}{2}L + 1$ to $\frac{3}{2}L$ to generate $|\Psi_{jj'}\rangle$, and on the regions of the above sites and the sites from $\frac{3}{2}L + 1$ to $\frac{1}{2}L$ separately so as to generate $|\Psi_{jj'}^p\rangle$. As will be elucidated in detail, U_{adj} involves two different expressions, $U_{adj}^{(1)}$ and $U_{adj}^{(2)}$; the latter takes the form of $U_{adj}^{(2)} = \sum_j |\psi_j^p\rangle\langle\psi_j^{\circlearrowleft}|$, in which $|\psi_j^{\circlearrowleft}\rangle \equiv \hat{\mathcal{T}}^{L/2}|\psi_j\rangle$ denotes a state through translating $|\psi_j\rangle$ by $L/2$ sites and $\hat{\mathcal{T}}|i_L\rangle = |i_1\rangle$ has been assumed.

The theoretical foundation of the above formulated prescription rests on the following analysis about the utmost case in which the size L of the block is sufficiently large so that the system H_L can be viewed as thermally extensive. By dividing the block into two subsystems with intermediate coupling, $H_L = h_l + v_{lr} + h_r$, one can make an assertion that the low-lying spectra of H_L and of the disconnected Hamiltonian $h_l + h_r$ are identical: $E_n = E_{n_1}^l + E_{n_2}^r$, where $E_{n_1}^l$ and $E_{n_2}^r$ denote the spectra of the left half h_l and of the right half h_r, respectively. This is simply understood since the partition function of the block, $\mathbf{Z} \equiv \text{Tr}e^{-\beta H_L}$, should fulfill $\mathbf{Z} = \mathbf{Z}_l\mathbf{Z}_r$ for any finite temperature $1/\beta$; the latter identity, in which $\mathbf{Z}_{l,r} = \text{Tr}e^{-\beta h_{l,r}}$, actually accounts for the additivity of thermodynamic potentials of macroscopic thermal systems. As H_L and $h_l + h_r$ possess the same low-lying

spectra, the low-energy portion of the two systems could be linked by an isometry map, which turns out to delineate the first form of the prescribed transformation: $U_{adj}^{(1)} = \sum_n |\psi_n\rangle\langle\varphi_n|$, with $|\varphi_n\rangle \equiv |\varphi_{n_1 n_2}\rangle$ denoting the low-lying eigenstates of $h_l + h_r$. That is, the low-energy portion of H_L could be obtained via $U_{adj}^{(1)}(h_l + h_r)[U_{adj}^{(1)}]^\dagger$, and the effect of the intermediate coupling v_{lr} hence is equally described by the transformation $U_{adj}^{(1)}$.

It is then crucial to note that the formally range-L $U_{adj}^{(1)}$ indeed has an effective range less than L as the block size L increases asymptotically. Especially, for the infinite H_L with a gapped ground state, the range of $U_{adj}^{(1)}$ turns out to be local since the evolution operator generated by H_L in a finite period τ, formed as $e^{-ih_l\tau} \otimes e^{-ih_r\tau}$ sandwiched by $U_{adj}^{(1)}$ and $[U_{adj}^{(1)}]^\dagger$, could be simulated by a quantum circuit [11] with finite depth. The latter representative, which describes the time evolution operator in virtue of a few layers of piecewise local unitary operators, has also been exploited to characterize quantum phases and topological orders for quantum many-body systems [12, 13].

Consequently, one can employ $U_{adj}^{(1)}$ further to connect the pair of Hamiltonians H_L^p and $H_L^\circlearrowleft \equiv H_L^p - v_{lr}$, in which $H_L^\circlearrowleft$, with edges inside the block, is simply a Hamiltonian achieved via translating H_L by $L/2$ sites. An additional condition to simulate the effect of v_{lr} here is that the effective range of $U_{adj}^{(1)}$ should be less than L, i.e., $U_{adj}^{(1)}$ should commute with v_{rl}. The second form of U_{adj}, $U_{adj}^{(2)} = \sum_j |\psi_j^p\rangle\langle\psi_j^\circlearrowleft|$, is then yielded and the contained $|\psi_j^\circlearrowleft\rangle$ are just eigenstates of $H_L^\circlearrowleft$. By the same token, as the compound systems H_{2L} and H_{2L}^p are considered, the effects of interblock couplings v_{12} and v_{21} on their low-energy behavior could be simulated by imposing the transformations, either $U_{adj}^{(1)}$ or $U_{adj}^{(2)}$, on corresponding adjacent segments of the disconnected system $H_L^{[1]} + H_L^{[2]}$.

The analysis above reveals that the regularized basis sets of equations (1) and (2), or more accustomedly, their symmetric and anti-symmetric combinations $|\Psi_{J\pm}\rangle \equiv |\Psi_{jj'}\rangle \pm |\Psi_{j'j}\rangle$ and $|\Psi_{J\pm}^p\rangle \equiv |\Psi_{jj'}^p\rangle \pm |\Psi_{j'j}^p\rangle$, specify exactly the low-energy solutions for compound blocks H_{2L} and H_{2L}^p as $L \to \infty$. It thus illuminates a regularized version of the NRG scheme by incorporating the described transformation into the algorithm in order to reconstruct Hamiltonians for doubly increasing blocks. Historically, the speculation through applying a variety of boundary conditions to perform the NRG procedure has ever been endeavored by White and Noack in dealing with the tight-binding model and the localization problem of one dimension [7, 14]. The discovery of the distinct prescription here should enable us to exploit the NRG method for general quantum lattice systems, i.e., for interacting systems and for systems with high spatial dimensions.

The key of the present algorithm rests on recognizing correspondences among basis states of the Hamiltonians with different boundary configurations so as to build the transformation U_{adj}. For this purpose, one should separate the basis states by quantum numbers and then discern the matching of states among different sets but with identical quantum numbers through comparing their fidelities. Due to finite-size effects, the matching of states would become less evident as the energy level increases; it requests consequently that the initial block to be exactly diagonalized should be of considerable size. It should be noted that, in spite of the correspondences having been established, U_{adj}'s are still not uniquely determined owing to the phase uncertainty of the eigenstates. This uncertainty, however, doesn't affect the basic efficiency of the scheme since different choices of the phases have no influence on the transformations under $L \to \infty$. In practical calculations it can be simply removed, e.g., by setting $\langle\psi_k|\varphi_k\rangle$ (or $\langle\psi_k^\circlearrowleft|\psi_k^p\rangle$) to be real and positive [15].

To verify the efficiency of this new version of the NRG scheme, the algorithm has been implemented to calculate a periodic spin-1 antiferromagnetic Heisenberg model $H = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$ with 16 sites. The initial H_L and $h_l + h_r$ with $L = 8$ are exactly diagonalized and the transformation $U_{adj}^{(1)}$ is employed to generate the basis states for H_{2L}^p. The algorithm recovers the exact energy [16, 17] to at least 5 digits (with $m = 47$ or more states to be kept). As the derived low-lying spectra are shown in Table I, some key points to perform the algorithm are recited as below. (1) It is convenient to invoke four-component tensors to represent the states: $|\psi_j\rangle \otimes |\psi_{j'}\rangle \equiv \psi_{j_l j_r j_l' j_r'}$, where the indices j_l, j_r, j_l' and j_r' account for the four half blocks with size $L = 4$, respectively. Transformation of U_{adj} on adjacent halves is then realized by summations over indices (j_r, j_l') or (j_r', j_l). (2) Symmetries related to the total spin S^2 and S_z can be exploited to reduce the computing cost since these invariants are preserved under the transformation U_{adj}. States with definite quantum numbers (s, s_z) for the $L = 16$ block are readily con-

TABLE I: Energies of 21 low-lying states of the $L = 16$ Heisenberg chain obtained by the regularized NRG scheme using $U_{adj}^{(1)}$. Presented also includes the information of the degeneracy f, quantum numbers of the total spin s and the momentum k of the corresponding energy levels yielded by the symmetry-preserved algorithm. An accuracy about 10^{-5} is obtained by keeping $m = 47$ states (cf. the values of the ground and the first-excited energies achieved by exact diagonalization $E_0 \approx -22.44681$ and $E_1 \approx -22.00401$ [16, 17]).

	$s; k$	$m = 21$	$m = 47$
E_0 $(f = 1)$	$s = 0; k = 0$	-22.44170	-22.44639
E_1 $(f = 3)$	$s = 1; k = 8$	-21.99120	-22.00326
E_2 $(f = 6)$	$s = 1; k = 7, 9$	-21.36381	-21.37456
E_3 $(f = 5)$	$s = 2; k = 0$	-21.27190	-21.28826
E_4 $(f = 6)$	$s = 1; k = 1, 15$	-21.06151	-21.07610

structed by those of $L = 8$ in virtue of Clebsch-Gordan coefficients [18], which are then acted on by the transformation $U_{adj}^{\otimes 2}$ and are Gram-Schmidt orthonormalized afterwards so as to get the desired basis states, $|\Psi_{J,s,s_z}^p\rangle$. (3) The algorithm described till now does not involve the translational symmetry except for that of the blocked translation with 8 sites. To cope with the full translational symmetry, one should construct states with definite momentum quantum number k using the basis states $|\Psi_{J,s,s_z}^p\rangle$ and $\hat{\mathcal{T}}^i|\Psi_{J,s,s_z}^p\rangle$ ($i = 1, \cdots, 7$), and then diagonalize the Hamiltonian H_{2L}^p in symmetry-preserved spaces with quantum numbers (s, s_z, k).

Extensions of the proposed NRG scheme to lattices with more than one spatial dimension could be naturally procured. Take the square lattice as an example: by sketching out four different boundary configurations of an $L \times L$ lattice [see Fig. 1 (a) and (b)], the transformations $U_{adj}^{(1)}$ and $U_{adj}^{(2)}$ could be constructed from eigenstates of pair configurations, either (i) and (ii) of Fig. 1 (a) or (iii) and (iv) of Fig. 1 (b), respectively. Since the lattice Hamiltonian usually possesses symmetries related to a specific crystallographic point group, classifying degenerate eigenstates via irreducible group representations [19] should be a task prerequisite to the procedure. The compound system of the quadrupled block needs to be represented by a 16-component tensor with indices illustrated in Fig. 1 (c). Basis states for the block Hamiltonian with periodic boundary conditions are obtained by imposing U_{adj} on each joining region with fourfold adjacent edges, which can be realized via summations over corresponding indices, respectively.

As a test case, the two-dimensional scheme is examined by a tight-binding model, a single particle hopping on a square lattice with a Hamiltonian

$$H = \sum_{x,y}[(ua_{x+1,y}^\dagger a_{x,y} + h.c.) + (va_{x,y+1}^\dagger a_{x,y} + h.c.)], \quad (3)$$

where $a_{x,y}^\dagger$ and $a_{x,y}$ are the creation and annihilation operators on the site (x, y) and the hopping parameters are set as $u = -1$ and $v = -3/2$. The Hamiltonians of an $L = 64$ square lattice with various boundary configurations are exactly diagonalized of which the eigenstates of configurations (ii) and (iv) are recorded as $|\psi_j\rangle$ and $|\psi_j^p\rangle$, respectively. Unitary U_{adj}'s can be built for the present system through full correspondences of the derived bases, which enables us to calculate states for the quadrupled lattice at any energy level. Starting from m states $\{|\psi_j\rangle\}$ closest to a particular energy, the $4m$ basis states of the compound periodic lattice are generated and divided into four sets, $\{|\Psi_j^{\pm,\pm}\rangle, j = 1, \cdots, m\}$, in which "$\pm$" denotes the symmetric or anti-symmetric property of states under $\hat{t}_{x(y)} \equiv \hat{\mathcal{T}}_{x(y)}^L$, translations along the x (y) direction by L sites. The lowest energies of the $L = 128$ system achieved by the algorithm via $U_{adj}^{(1)}$ are shown in Table II, with which the exact energies and the energies achieved
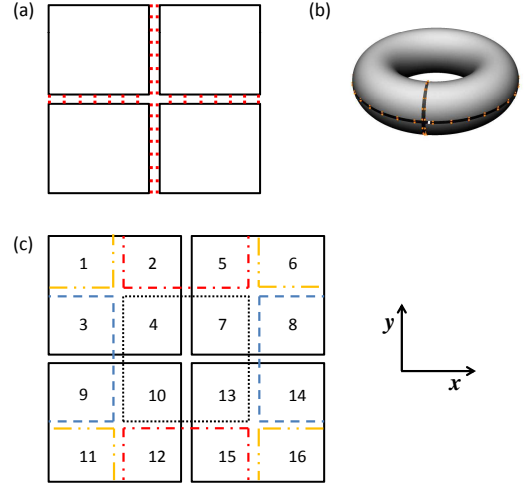

FIG. 1: Schematic of configurations of the square lattice. (a) Configurations (i) and (ii) of the $L \times L$ lattice with open boundaries, in which inside edges are either disconnected [configuration (i)] or connected [configuration (ii)]. (b) Lattice configurations (iii) and (iv) with connected boundaries. The one with disconnected inner edges [configuration (iii)] is equivalent to the configuration (ii) up to a translation along both x and y directions by $L/2$ sites. (c) Configuration of the representative tensor for the compound quadrupled lattice. The joining regions of adjacent segments are indicated by indices $\{4, 7, 10, 13\}$, $\{8, 3, 14, 9\}$, $\{12, 15, 2, 5\}$, and $\{16, 11, 6, 1\}$, on which U_{adj} should be imposed separately.

by the primitive NRG are presented for reference.

Performance of the algorithm employing the prescription $U_{adj}^{(2)}$ on the above two models, the spin-1 Heisenberg chain and the tight-binding model, displays that it is slightly less accurate than that utilizing $U_{adj}^{(1)}$. For example, the algorithm using $U_{adj}^{(2)}$ yields a ground-state energy $E_0 \approx -22.43222$ for the 16-site Heisenberg chain provided that the same amount of 47 states are kept. Nevertheless, it is of interest to mention an exceptional case of the tight-binding model, where the numerical calculation discloses that the symmetric basis states $\{|\Psi_j^{+,+}\rangle\}$, generated via imposing $U_{adj}^{(2)}$'s on the state vectors of direct sum $|\psi_j\rangle \oplus |\psi_j\rangle \oplus |\psi_j\rangle \oplus |\psi_j\rangle$, are exact eigenstates of the quadrupled system with periodic boundary conditions. In view that the intercepted state vector of any joining segments with fourfold adjacent edges represents a basis state of the lattice configuration (iii), the transformation $U_{adj}^{(2)}$ on each of those joining segments maps it precisely onto $|\psi_j^p\rangle$, a basis state of the lattice configuration (iv). That is to say, direct combinations of basis states of the periodic $L \times L$ block, $|\psi_j^p\rangle \oplus |\psi_j^p\rangle \oplus |\psi_j^p\rangle \oplus |\psi_j^p\rangle$, already give rise to one fourth of the full set of exact solutions of the compound $2L \times 2L$ system. This result is indeed general: it is independent of the size L and applies also to the one-dimensional tight-binding model wherein it is

TABLE II: Lowest energies of the $L = 128$ square lattice with periodic boundary conditions achieved by the regularized NRG algorithm via the prescription $U_{adj}^{(1)}$. The energies are calculated in separated spaces of the four sets of basis states $\{|\Psi_j^{\pm,\pm}\rangle, j = 1, \cdots, m\}$ with $m = 64$ and are listed according to their values. The results recover the exact energies to 4-5 digits and exhibit correct order, while the results obtained by the primitive NRG scheme are quite inaccurate and fail to yield the same ordering.

	$\{\hat{t}_x, \hat{t}_y\}$	Exact	Regularized RG	Primitive RG		$\{\hat{t}_x, \hat{t}_y\}$	Exact	Regularized RG	Primitive RG
E_0	$\{+,+\}$	-5.00000	-4.99960	-4.99462	E_8	$\{-,-\}$	-4.99398	-4.99386	-4.97853
E_1	$\{-,+\}$	-4.99759	-4.99732	-4.99431	E_9	$\{+,+\}$	-4.99037	-4.99011	-4.98698
E_2	$\{-,+\}$	-4.99759	-4.99728	-4.98821	E_{10}	$\{+,+\}$	-4.99037	-4.99009	-4.98314
E_3	$\{+,-\}$	-4.99639	-4.99623	-4.99417	E_{11}	$\{+,-\}$	-4.98676	-4.98674	-4.98494
E_4	$\{+,-\}$	-4.99639	-4.99617	-4.98653	E_{12}	$\{+,-\}$	-4.98676	-4.98672	-4.97730
E_5	$\{-,-\}$	-4.99398	-4.99395	-4.99387	E_{13}	$\{+,-\}$	-4.98676	-4.98668	-4.97698
E_6	$\{-,-\}$	-4.99398	-4.99391	-4.98776	E_{14}	$\{+,-\}$	-4.98676	-4.98666	-4.96774
E_7	$\{-,-\}$	-4.99398	-4.99389	-4.98463	E_{15}	$\{+,+\}$	-4.98555	-4.98541	-4.97742

very easy to verify.

In the present algorithm at least two truncated basis sets are kept and they should be expressed in a complete set of spin bases. This should be the case at each iteration since any such truncated set is too incomplete to represent other basis states with different boundary configurations. As a result, repetition of the described RG procedure is constrained by the capacity of storing vectors with exponentially growing dimensions. In this sense, the regularized NRG scheme is applicable to finite lattices rather than the infinite one since the iterative performance of the procedure for the latter system will break down inevitably. This indeed offers the underlying cause which supports partly the folklore stating that all real-space RG schemes are necessarily inaccurate for lattice systems.

Alternatively, if one chooses to sacrifice some of the accuracy, an iterative procedure could be achieved, at least for one-dimensional systems, by projecting the derived basis states, e.g., those of H_{2L} and H_{2L}^p, on the tensor product space of the m states kept to get bases $|\tilde{\psi}_j\rangle$ and $|\tilde{\psi}_j^p\rangle$ of dimension m^2. The prescribed transformation, $\tilde{U}_{adj}$, could be built by virtue of these basis states which is then imposed on the states $|\tilde{\psi}_j\rangle \otimes |\tilde{\psi}_{j'}\rangle$ to generate basis states for the pair of Hamiltonians with larger size. The truncation of the algorithm here is distinctly different from that of the primitive NRG scheme in view that the m states kept are taken from a Hilbert space of dimension m^4 instead of dimension m^2. It is also worthy to note that the strategy adopted here, projecting the basis states of the compound block onto a restricted space of tensor product states of subsystems, is what has been done in the contractor RG method [20–22]. In comparison, the interblock coupling of the effective Hamiltonian in the latter scheme is obtained by substracting the contributions of contained subclusters, while in the present scheme the effective Hamiltonian of the compound system could be constructed directly by virtue of the regularized basis states.

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